CS 450: Numerical Anlaysis

Chapter 1 – Scientific Computing

Lecture 1

Numerical analysis introduction, motivation, and applications

Posedness, error, and conditioning

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Scientific Computing Applications and Context

- **Mathematical modelling for computational science** *Typical scientific computing problems are numerical solutions to PDEs*
  - *Newtonian dynamics: simulating particle systems in time*
  - *Fluid and air flow models for engineering*
  - *PDE-constrained numerical optimization: finding optimal configurations (used in engineering of control systems)*
  - *Quantum chemistry (electronic structure calculations): many-electron Schrödinger equation*
- **Linear algebra and computation**
  - *Linear algebra and numerical optimization are building blocks for machine learning methods and data analysis*
  - *Computer architecture, compilers, and parallel computing use numerical algorithms (matrix multiplication, Gaussian elimination) as benchmarks*

Example: Mechanics[1]

- Newton's laws provide incomplete particle-centric picture
- Physical systems can be described in terms of *degrees of freedom* (DoFs)
  - A piston moving up and down requires 1 DoFs
  - 1-particle system requires 3 DoFs
  - 2-particle system requires 6 DoFs
  - 2-particles at a fixed distance require 5 DoFs
- N-particle system *configuration* described by $3N$ DoFs

[1] *Variational Principles of Mechanics*, Cornelius Lanczos, Dover Books on Physics, 1949.

Course Structure

- **Complex numerical problems are generally reduced to simpler problems**

eigenvalue problems → linear systems

PDEs → algebraic equations

optimization → nonlinear solve

↳ linear systems

- **The course topics will follow this hierarchical structure**

representation:

floating point

analysis:

error & conditioning

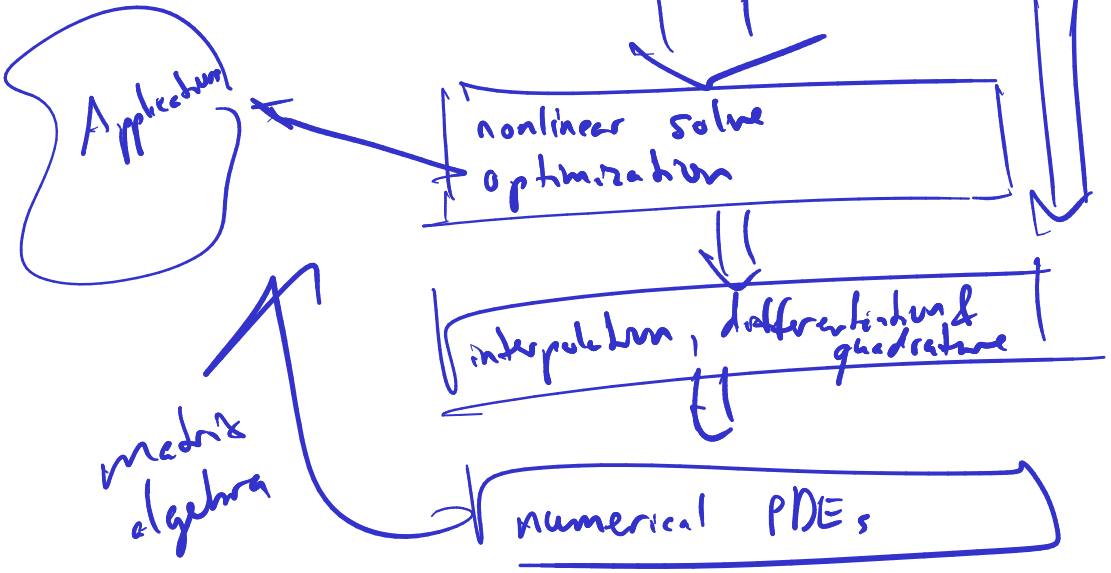
→

matrix algebra

linear systems

↘ least squares

↘ eigenvalue problems


Application
nonlinear solve
optimization
interpolation, differentiation & quadrature
matrix algebra
numerical PDEs

Numerical Analysis

- **Numerical Problems involving Continuous Phenomena**:

as opposed to discrete

solve $f(x)$ for input x, so

$f(\hat{x}) \to f(x)$ as $\hat{x} \to x$ well-posed

if not ill-posed

- **Error Analysis**:

error vs complexity

Absolute error: approx. soln − exact : $\hat{f}(x) - f(x)$

Relative error: $\frac{\text{absolute error}}{\text{exact soln}}$: $\frac{\hat{f}(x) - f(x)}{f(x)}$

Vector quantities $v \in \mathbb{R}^n$

$f(v) \in \mathbb{R}$

error $\dfrac{\hat{f}(v) - f(v)}{\|v\|}$

Sources of Error

- **Representation of Numbers:** how do we represent a real number?
  Scientific notation (significant digits)
  3.14×10^0 1.011×2^3
  precision → number of represented significant digits
  ≠ accuracy | error $f(x) - x$
- **Propagated Data Error:**
  error introduced at/before input
  e.g. experimental measurements
- **Computational Error** = $\hat{f}(x) - f(x)$ = **Truncation Error** + **Rounding Error**
  approximation error made by algorithm

Error Analysis

- **Forward Error**:

absolute & relative

given input x, true solution $f(x)$
computed solution $\hat{f}(x)$

forward error if $\hat{f}(x) - f(x)$

- **Backward Error**:

$\Delta x = \hat{x} - x$ where $f(\hat{x}) = \hat{f}(x)$

min Δx such that ↑

relative backward error would be $\frac{\hat{x} - x}{x}$

Conditioning

- **Absolute Condition Number**:

$$\lim_{|\Delta x| \to 0} \max_{\text{perturbations}} \max_{\text{inputs} \in \text{range}} \frac{|\text{perturbation to output}|}{|\text{perturbation to input}|}$$

$$\lim_{|\Delta x| \to 0} \max_{\Delta x} \max_{x \in \text{inputs}} \frac{|f(x+\Delta x) - f(x)|}{|\Delta x|}$$

for $f(x)$ at x

$$\lim_{h \to 0} \left| \frac{f(x+h) - f(x)}{h} \right|$$

- **(Relative) Condition Number**:

conditioning w.r.t. relative error

if inputs $= [0,1]$

$$E_{abs} = \max_{x \in [0,1]} |f'(x)| = |f'(x)|$$

e.g. for $f(x)$ at x

$$E_{rel} = \left| \frac{f'(x) \cdot x}{f(x)} \right|$$

Posedness and Conditioning

- **What is the condition number of an ill-posed problem?** ∞

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forward error vs backward error

given bound on conditioning κ
and we find a b-ckward error bound of $|E|$
We have forward error bound $\kappa \cdot |E|$

Stability and Accuracy

- **Accuracy**: how far away we are from desired soln.
- **Stability**: sensitivity of algorithm to perturbations/approx